The CCP13 FibreFix Program Suite and Recent Updates

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Abstract

Many users are currently applying the new CCP13 software package FibreFix to their own research. This is both testing the software under varied real world conditions and also, in some cases, leading to requests for the software to be modified or enhanced for the specific needs of the user. So, both through user requests, the correction of bugs, and the already planned enhancement of FibreFix, a number of changes have been made to the original FibreFix suite both to improve it and to make it more powerful. These changes are implemented in the current version (FibreFix 1.3). They include addition of new 'BSL' operations and improvement in the input and control of some of the original BSL functions. We outline these developments here.

Following the initiation of CCP13 in the early 1990s, a number of independent programs were developed, particularly by Dr. Richard Denny, to process and analyse data in non-crystalline diffraction patterns (Denny, 1993; Denny and Shotton, 1999; Denny et al., 1998). These programs, the most important of which in their latest incarnations are termed XCONV, XFIX, FTOREC and LSQINT, were designed to build on the existing BSL program developed by Joan Bordas and Geoff Mant at the Daresbury Laboratory. They were built around what became the standard BSL file format. All of these programs were written for UNIX platforms and, although being very effective, they were rather non-intuitive and cumbersome in their use. The CCP13 Committee therefore decided to link these programs in an integrated, user-friendly, suite firstly in a PC Windows environment. In addition, the original programs required parameters determined in one process to be carried forward manually into the next routine, a rather laborious process. The new program suite was therefore required to integrate the original programs into a single 'suite' where parameters that have already been determined in one part of the analysis are automatically carried forward to the next without user intervention (Squire et al., 2003). The resulting suite, originally known as ICE but now called FibreFix, is implemented for the Microsoft Windows platform (He et al., 2004; Rajkumar et al., 2005). It includes the functionality of the programs XCONV, XFIX, FTOREC and LSQINT and also all of the routines which were originally part of the UNIX BSL program. It is intended that the whole FibreFix suite will eventually be ported to Java, or an equivalent platform, so that it can also be used on any UNIX or LINUX machine.

Here we describe a number of new features that have been implemented in the current FibreFix program (FibreFix Version 1.3) and we discuss planned future developments.

Loading of files

The program XCONV was originally the way of converting images from detector format into the BSL format used by the CCP13 software. Loading an image was often an interactive process. FibreFix has now been developed so that the XCONV functionality is automatically present. Image files in known formats can either be loaded using the normal 'open' function under the 'file' drop down menu, or can simply be 'dragged and dropped' into the image window. The FibreFix program automatically recognises many standard detector formats and image formats and will open the files automatically without user interaction unless there are some uncertainties in, for example, the image array size. As discussed later (Figure 6), several image files can easily be loaded at the same time and can be treated as successive 'frames' of a single image.

Improvements and updating of 'old' BSL functions in FibreFix 1.3

Many of the old BSL functions have been implemented in FibreFix and in several cases improved. Initially FibreFix created plots using the BSL functions HOR (integrate HORizontally), VER (integrate VERtically), SEC (SECtor integration), RIN (Radial INtegration) and TIP (Time series Intensity Plot) by selecting appropriate regions of the diffraction pattern using the mouse, then right clicking on the mouse to display the plot in a new
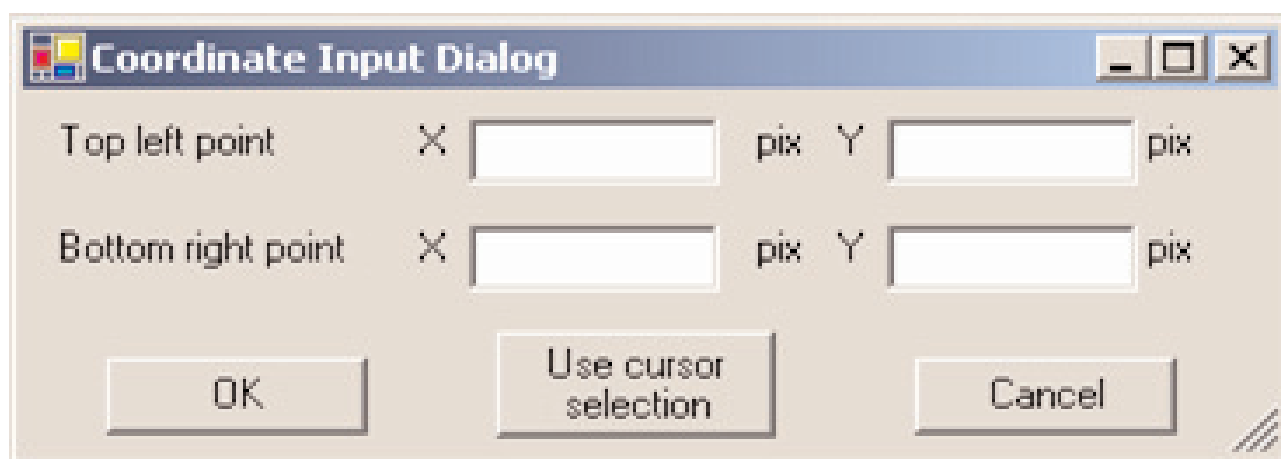
Figure 1: The new query box which appears when it is necessary to select precise parameter ranges for intensity integrations in FibreFix.

popup window. However, it was difficult to be precise in positioning the mouse to select an exact area of the image, especially if it is necessary to analyse the same regions in many different patterns using the same limits of integration. These plot regions can now be selected in an alternative way by entering the exact pixel coordinates of the area for integration in a popup window as shown below (Figure 1). Clicking on OK will plot the graph in a separate popup window as before.

Another development is such that the program plotting functions have been updated to plot one-dimensional logs when the image is displayed in a log scale. Also a number of bugs in these routines have been fixed.

New BSL functions in FibreFix
FibreFix 1.3 has been updated with several new added BSL functions such as ADF (ADdition of a series of Frames), CAL (CALibration file normalisation) and CIN (Circular INtegration) which are used as below. There has also been a modification to the use of the ROTation function ROT:

[1] ADF: The ADF function adds sets of image Frames together in a time series. By specifying the Frames to be added in the input window, specific groups of Frames in a time series can be added together. Note that only where several Frames are being added is it necessary to include those Frame numbers in the ADF query box. In the example below (Figure 2) new Frame 1 is the same as old Frame 1, new Frame 2 is the sum of old Frames 2 to 4, new Frames 3 and 4 are replaced by old Frames 5 and 6, new Frame 5 is replaced by the sum of Frames 7 to 12 and so on.

As a separate application of the ADF function, several independent exposures (files) of exactly the same repeated experiment can be added together by inputting them as a set of files using the input procedure in Figure 6. They
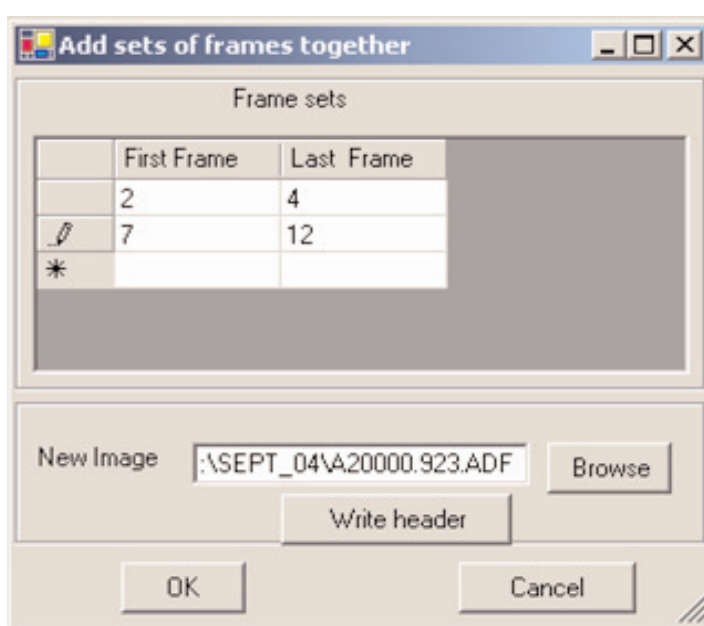

Figure 2: The query box which appears when using the BSL 'ADF' function in FibreFix.

are then stored in the program as if they are successive Frames in a multiframe file and can be added together using the ADF function.

[2] CAL: The CAL function plots a modified calibration file by dividing the calibration value for each frame by the user input exposure time of each frame in a time series. This allows the measurement which has been saved in the calibration file to be normalized with respect to exposure time so that a sensible plot can be made of the calibration data against frame number. In order to explain the application of CAL, we give an example below from one of our own time-resolved X-ray diffraction experiments on fish muscle (Figure 3). In the recorded exposures the frame duration changed as in Table 1:

[3] CIN: The CIN function plots circular integration profiles in a selected radial range of a diffraction pattern. By

Frames up to	Exp time (ms)
2	100
152	1
153	100
254	4

Table 1: *Frame numbers and exposure times in a time-resolved X-ray diffraction experiment on contracting bony fish muscle. Frames 1 and 2 each had exposure times of 100 ms, Frames 3 to 152 had exposure times of 1 ms, Frame 153 had an exposure of 100 ms, and Frames 154 to 254 had exposures times of 4 ms. These translate into the entry in the CAL function input query box in BSL as in Figure 3.*
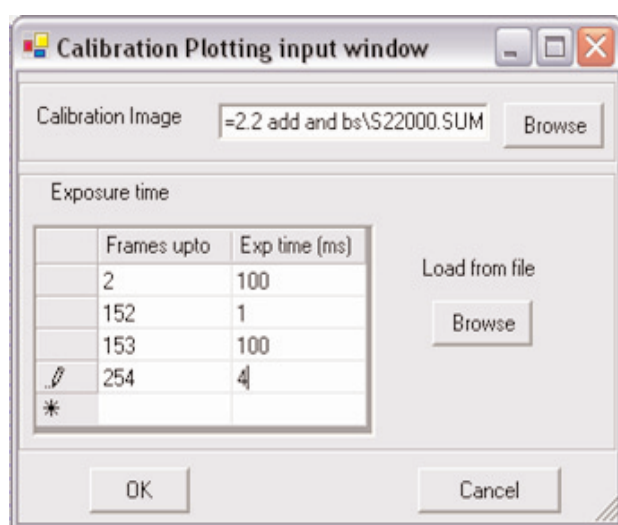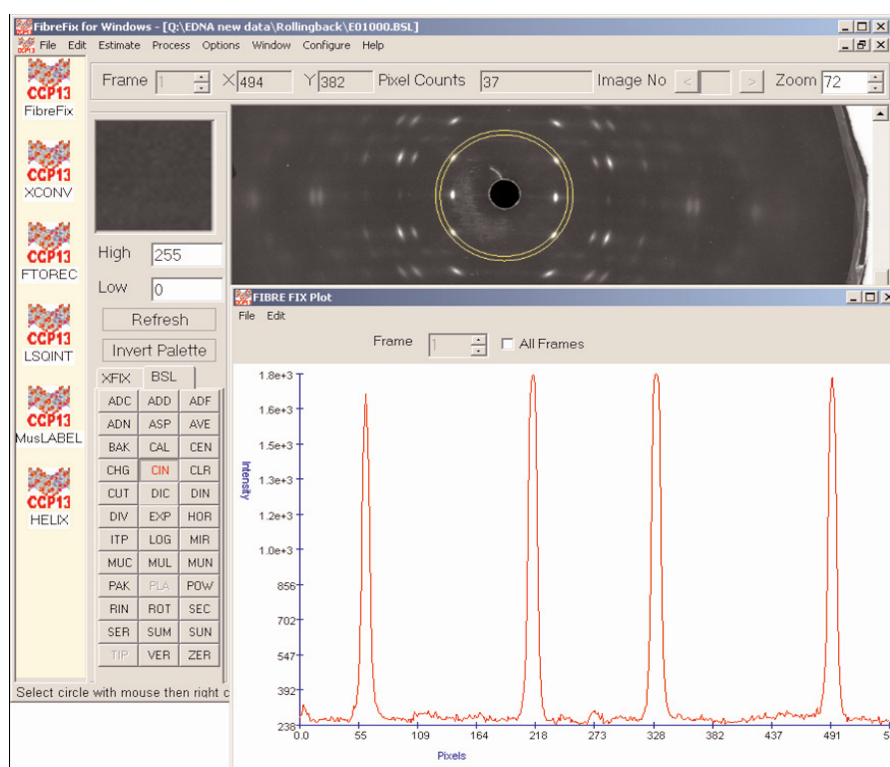

Figure 3: *The query box which appears when using the BSL 'CAL' function in FibreFix.*

Figure 4: *Application of the new BSL 'CIN' (circular integration) function in FibreFix. This selects and plots the observed intensity around an annulus in the observed diffraction pattern and can reveal details of the degree of orientation in a polymer sample.*
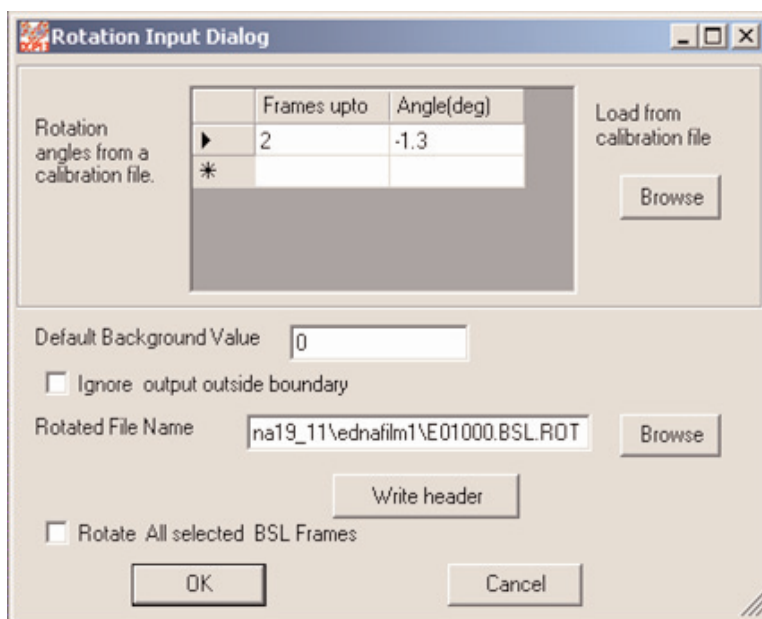
Figure 5: The new query box that appears when the BSL function 'ROT' is opened. It allows for variable correction of the pattern rotations throughout a time-series.
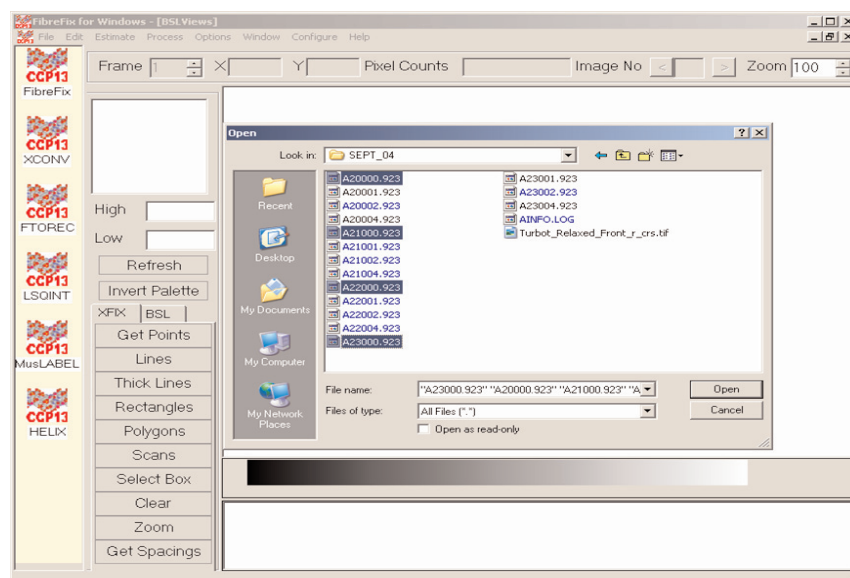
selecting the CIN function on the BSL tool tab one can plot the required intensity profile around a circle either by mouse clicking or by inputting the centre, radius and radial width of the annular area to be integrated. Then by right-clicking on the mouse the annular intensity profile is plotted (Figure 4). This can be used, for example, for estimating the degree of orientation (texture) in partially ordered synthetic polymer samples.

[4] ROT: The ROT tool has been updated to allow for slight variations in absolute orientation of the fibre axis of a single sample during a time series. It applies different angles of rotation to different time frames (Figure 5).

Multiple files can be selected and processed together
Multiple files can be selected in FibreFix and operations can then be carried out on all the files selected as the mul-

tiframe BSL file. Multiple files can be selected by holding the CTRL key while clicking the necessary files (Figure 6). Alternatively files can be selected by clicking the first file to select and then, while holding down the SHIFT key, clicking the last file to select. The program assumes all the selected files are of same file format and the same dimensions.

Estimation of Spacings and Unit Cell Parameters
A new feature of FibreFix 1.3 is the ability to determine approximate peak spacings in the pattern once the wavelength and camera length have been put into the Parameter file. Using the Get Spacings option under XFIX, the user can click on a peak of interest of unknown spacing, right click and automatically generate spacing estimates. These are printed in the text box at the bottom of the FibreFix window. The estimated 'real' spacings given are the Bragg spacing d and, for 'vertically' oriented fibre specimens, the radial (row line) and axial (layer line) spacings of the peak. From these spacings the approximate dimensions of the unit cell can be defined.

Modelling Programs
As well as stripping fibre diffraction data and analysing other kinds of non-crystalline diffraction patterns, it is important to have tools with which to model possible candidate structures. Two simulation programs have been written, the program HELIX (Knupp and Squire, 2004) to model simple helical structures and also the program MusLABEL (Squire and Knupp, 2004) to model the specific kinds of structures that are found in striated muscles. The least-squares molecular refinement program LALS is also in the process of being updated for CCP13 (Arnott et al., 1969).

Figure 6: Selection of multiple files for common processing within BSL.

The future: Proposed additional updates

In the near future a number of additional features will be added to FibreFix.   These include additional routines within the BSL processing package such as:

CNV   **Co**N**V**olute two files.

CON   Generate a **CON**tour map.

FFT   Perform 2-D Fast Fourier Transform on an image.

GAU   Generate a 2-D **GAU**ssian function.

IFT   Calculate the **I**nverse **F**ourier **T**ransform.

SUR   **SUR**face plot (isometric projection).

It is also hoped that new background subtraction procedures will be included in **FTOREC** and **LSQINT**.   The full program will also include a 2D or 3D Fourier synthesis package based on data output from **LSQINT**.

Finally we hope that before too long updated versions of the 1D analysis programs **XFIT** and **XOTOKO** will also be incorporated within **FibreFix**.   When we have a final package which we believe fulfils a great deal of the needs of the non-crystalline diffraction community we will implement the whole **FibreFix** suite in Java.   Please also note that there are several **FibreFix** tutorials on the CCP13 website (www.ccp13.ac.uk) which refer to particular kinds of user applications.

Acknowledgements

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